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PLENARY LECTURE

The nanostructure inverse problem in the time of artificial intelligence

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The nanostructure inverse problem (NIP) aims to answer the following question: given a diffraction pattern from a nanostructured material, what is the 3D arrangement of atoms that gave rise to it? It seems that it the same as the 'crystal structure inverse problem' that is (largely) solved by the powerful methods of crystallography. However, a number of aspects make this problem much more challenging. First, it is difficult or impossible to get a 3D pattern from a single nanoparticle or nanodomain often forcing us to solve the problem from nano-powder-data, which greatly degrades the information content in the data. Second, the resulting structural models are more complex than those from regular crystals because, beyond the location of atoms in a well-defined unit cell, it is necessary to specify the nature of aperiodic deviations from the average (for example, position dependent bond-lengths, surface relaxations and dressing, etc.), and to specify morphological aspects of the nanoparticles and nanodomains. The reduction in information content in the data, coupled with the increase in the complexity of the resulting models make these problems often ill-posed with no unique, correct, solution. Nonetheless, the fundamental importance of the structure-property relationship in materials means that solve this problem we must, and with picometer precision.

In this talk I will discuss some changes in approach to the problem that we have recently been exploring that take us in the direction of the use of data analytics, machine learning, and artificial intelligence. These approaches have had a powerful impact in commerce and our online life, but less so in materials science. The attraction of these approaches is that they are inherently well tuned to handle ill-posed statistical problems such as the NIP, but it will require a change how we approach the analysis of these problems. I will discuss our initial steps in this direction and propose a path forward.

Keywords: **pair distribution function; nanoparticles; nanomaterials; machine learning; AI**